Chemical life cycle alternative assessment as a green chemical substitution framework: A feasibility study

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一、 *前言* (Introduction)

Sustainable actions are needed more than ever worldwide, in a global partnership to improve quality of life and protect the environment. Recent efforts were made to reduce the use of harmful chemicals throughout product production and processes. Chemical Alternatives Assessment has proven to be a viable solution for chemical pollution management as it provides a great methodology to inform product design and filter out and substitute hazardous chemicals (Matlin et al., 2015). An integration of both current chemical alternatives assessment and life cycle assessment could deliver the best of both worlds in terms of screening out hazardous chemicals for greener alternatives (Whittaker, 2015). Through the amalgamation of both chemical alternatives assessment and life cycle assessment, a new framework can be developed that includes the quantification of the various exposures and life cycle impacts of chemical alternatives, utilizing the available technologies and research data to achieve better results in chemical substitution for a more sustainable system (Fantke et al., 2020). This study aims to propose a Chemical Life Cycle Alternative Assessment (CLiCAA) framework and then conduct a feasibility study a target chemical of tetrachloroethylene (perchloroethylene) and its possible alternatives including: Trichlorethylene, Benzene, O-xylene, Dichloromethane, and Toluene.

二、 研究方法 (Research methods)

The Chemical Life Cycle Alternative Assessment (CLiCAA) framework consists of a four-step assessment system that can be replicated and used for filtering and substituting a variety of chemicals, including new chemicals with little to no data. The mandatory steps are the very first two filtering layers of this framework as they provide the necessary substitution suggestions and notification of unacceptable and hazardous chemicals in terms of human health risks and environmental impact potential (Zimmerman et al., 2015; Tickner et al., 2019). The final two filtering layers on the other hand are optional steps that can be implemented to further filter out more chemical alternatives and especially bridge the gap in unavailable data, specifically the cancer potency data, through the analysis of similar chemical molecular structures to the alternatives' (Song et al., 2017). Figure 1 presents the overview of the framework.

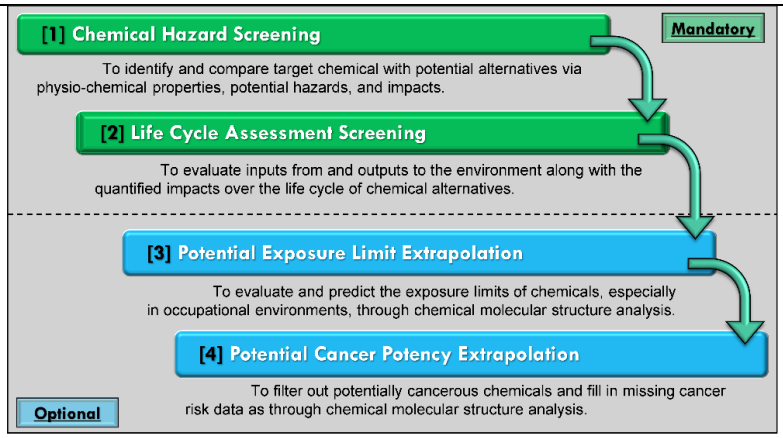

Fig 1. Overview of the CLiCAA Framework.

三、 結果與討論 (Preliminary Results and discussion)

In this feasibility study, the first set of chemicals have been analyzed with Tetrachloroethylene being the target chemical to replace. Going through the four layers in the CLiCAA framework, some preliminary results can be shared and discussed, as shown in Fig. 2 and Table 1.

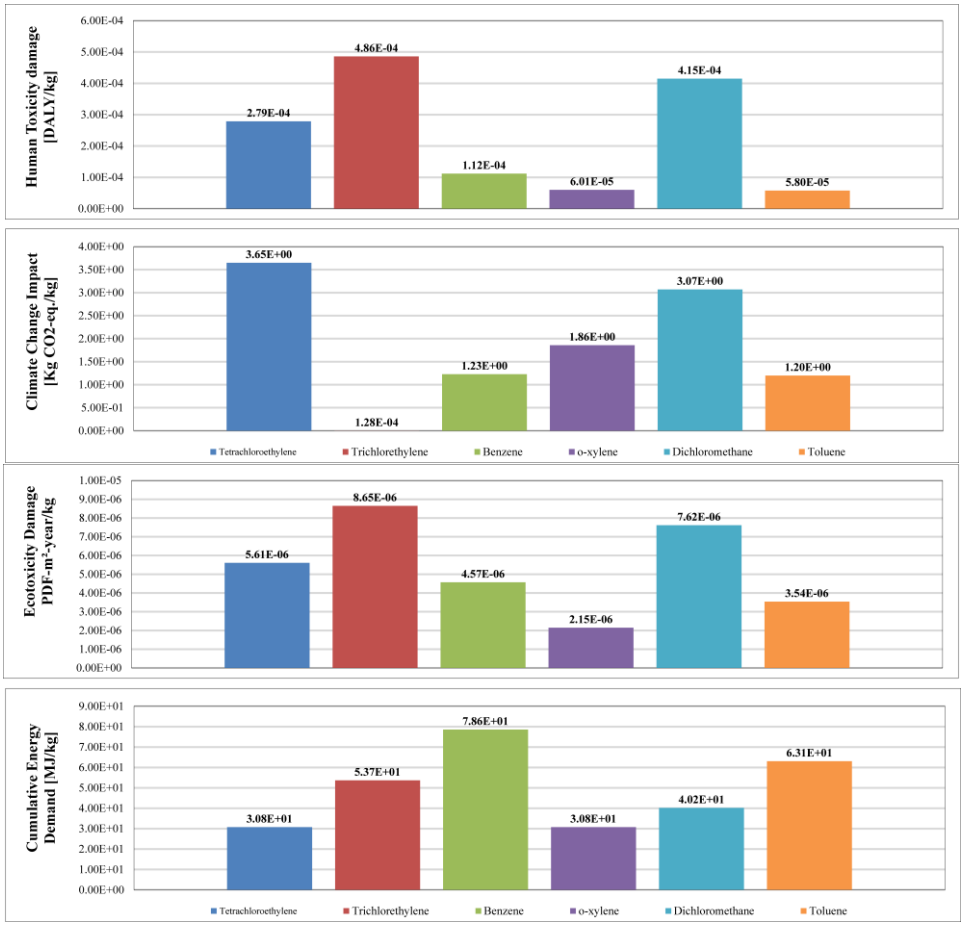

Fig 2. Life Cycle Assessment Screening results of chemicals' impact categories.

Through the first layer, Chemical Hazard Screening, Benzene appears to lack the necessary data for the human toxicity impact category, with Toluene lacking carcinogenicity studies, quantitatively. It is important to note that some chemicals such as o-xylene appear to have an advantage over Tetrachloroethylene. The Life Cycle Assessment Screening layer expands on the chemical alternatives in four impact categories whereby o-xylene and Toluene appear to be promising chemical alternatives to Tetrachloroethylene. Through the last two layers of the CLiCAA methodology, we can extrapolate missing data through the chemical molecular structure analysis of both o-xylene and Toluene, and use the estimated values as a reference to compare with Tetrachlorethylene. The Potential Exposure Limit Extrapolation layer explored the qualitative studies which suggest Toluene and O-xylene to have higher Reference Dose (RfD) and Reference Concentration (RfC) rates, which translate to higher exposure limits. This indicator highlights that chronic exposure to Tetrachloroethylene is more likely to result into much more serious health hazards than the two aforementioned alternatives. The Potential Cancer Potency Extrapolation layer has screened the alternatives along with "sister" chemicals that share similar molecular structure (Styrene, Cumene, and Ethylbenzene) with the potential alternatives (O-xylene and Toluene), in which all screened chemicals had no evidence of carcinogenicity. Giving both o-xylene and Toluene an edge over Tetrachlorethylene as their synopsis may be considered that of the full weight-of-evidence narrative.

The results from the feasibility study revealed that, for carcinogenic chemicals that lack cancer potency data being proven toxic, and providing a generally reliable guideline to understand and assess target and alternative chemicals for the best decision making.

Table 1. Summary on the chemical screening results for the studied chemicals

Chemical Screening	**Oral RfD (mg/kg-day)**	**Inhalation RfC (mg/m^3)**	**Oral CSF (mg/kg-day)**	**Inhalation CSF ($\mu g/m^3$)**
Tetrachloroethylene*	6.00E-03	4.00E-02	2.10E-03	2.60E-07
O-xylene	2.00E-01	1.00E-01	No Evidence	No Evidence
Toluene	8.00E-02	5.00E+00	No Evidence	No Evidence
Styrene^	2.00E-01	1.00E+00	No Evidence	No Evidence
Cumene^	1.00E-01	4.00E-01	No Evidence	No Evidence
Ethylbenzene^	1.00E-01	1.00E+00	No Evidence	No Evidence

^ are the sister chemicals that share similar molecular structure as both o-xylene and Toluene.
* is the target chemical to be replaced by a green alternative.

四、 結論 (Conclusions)

Throughout the layer implementations of CLiCAA, multiple firms can replicate the methodology to screen out the best chemical alternative for their own interest after integrating the framework with their Technical & Economic Feasibility Assessments among others. However, this framework is obviously not the best when it comes to high quality assessment of well-known chemicals as it does not cover up the entire supply chain of relevant chemicals throughout their life cycle, which requires additional resources and time to quantify and get to the full analysis. Yet it does aid well in understanding all kinds of chemicals in general, including those that have just been recently found and/or made thanks to the analysis of similar molecular structures and Life Cycle Assessment of the relevant chemicals.

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